

Butyl 2-hydroxy-2-methylpropanoate
816-50-2 | DTXSID50278111

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.91e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.52e-01

Confidence level: 6.78e-01

Nearest Neighbors from the Training Set

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Propan-2-yl 2-hydroxy-2-methylpropanoate

Measured: 1.03

Predicted: 5.47e-01

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Propyl 2-hydroxy-2-methylpropanoate

Measured: 6.84e-01

Predicted: 6.57e-01

Image not found

Pentyl 2-hydroxypropanoate

Measured: 6.24e-02

Predicted: 1.34e-01

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Butyl lactate

Measured: 2.74e-01

Predicted: 2.78e-01